

1,3-diphenyl-1,3-diazetidine
74949-76-1 | DTXSID60321268

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.18e-06 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.63e-01

Confidence level: 4.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Heptadecane,1-bromo-</div> <div>Measured: 9.00e-05</div> <div>Predicted: 1.98e-05</div>	<div>Image not found</div> <div>4-Aminoazobenzene</div> <div>Measured: 7.00e-08</div> <div>Predicted: 1.49e-06</div>	<div>Image not found</div> <div>C.I. Disperse Blue 1</div> <div>Measured: 8.45e-08</div> <div>Predicted: 1.43e-08</div>
<div>Image not found</div> <div>Isouron</div> <div>Measured: 1.20e-06</div> <div>Predicted: 1.37e-06</div>	<div>Image not found</div> <div>Pentylcyclohexane</div> <div>Measured: 2.00e-06</div> <div>Predicted: 6.06e-01</div>	